Master 2: *International Centre for Fundamental Physics*
INTERNSHIP PROPOSAL

Laboratory name: Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie
CNRS identification code: IMPMC – Sorbonne University
Internship director'surname: A. Marco SAITTA – PR Classe Exceptionnelle
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Internship codirector'surname: Michele Casula – CR IMPMC (SU)
Internship location: IMPMC – SU – Campus Pierre et Marie Curie
Thesis possibility after internship: YES
Funding: Likely (Labex/Idex/ANR), or ED's If YES, which type of funding:

Quantum^2 dynamics of water through machine learning

Water is the liquid of life. Fair enough! However, despite its tremendous importance for processes ranging from ion solvation to protein folding, not to speak of chemical reactions and even planetary science, a fully consistent description of water that builds from the fundamental interactions between hydrogen, oxygen and their surrounding electrons is still lacking. It is known that in order to have a reliable description of water, it is necessary to include quantum nuclear effects, whose motion must develop on the top of accurate potential energy surfaces (PES), provided by the solution of the electronic problem at given nuclear coordinates. We have recently developed an innovative method, which couples the accurate determination of the PES by quantum Monte Carlo methods with the quantum description of nuclei, treated as extended objects and not like point-like particles. The results on protonated water clusters are spectacular, as they indicate major quantum effects in proton transport at room temperature. However, the computational cost of this approach makes it difficult to study fully quantum^2 (quantum square!) bulk water.

In this master project, we propose to adapt machine learning techniques to analyse our quantum^2 dynamics of water clusters, and fit new interatomic potentials, with the aim of running the first quantum^2 dynamics-based simulation of bulk water. Machine learning methods are more and more used to improve interatomic potentials to spectacular accuracy, quantum^2 dynamics is known for its highest reliability. Merging together these two worlds for the first time will allow us to draw an unprecedented picture of water.

M. Dagrada et al., JCTC 10, 1980 (2014) ; F. Mouhat et al., JCTC 13, 2400 (2017) ;
F. Mouhat et al., in preparation (2018).

We look for a student strongly determined to undertake this ambitious and potentially breakthrough project, within a young and dynamical team.

Techniques in use: DFT, Quantum Monte Carlo, inference
Applicant skills: strong background in statistical mechanics, solid-state physics and/or physical chemistry, propensity for simulations and/or programming
Key words: theory, electronic structure, statistical mechanics, water, simulations
The team (scan the codes, see what we look like "in action"):
A. Marco Saitta, Full Sorbonne U Professor of Physics, team leader

Video from my General Seminar at the Physics Department of ENS, February 2015

Michele Casula, Chargé de Recherche CNRS at IMPMC, expert of Quantum Monte Carlo/Advanced Electronic Structure/Electronic Correlation

Video from my course at the Paris International School on Advanced Computational Materials Science, August 2015

Recent Publications: Besides the above-mentioned articles, our team has a consolidated expertise and a strong publication record in the development of advanced approaches, successfully applied to the study of molecular systems, including 7 PNAS, 2 Nature Comm and 8 PRL in the last few years.

Condensed Matter Physics: YES	Macroscopic Physics and complexity: YES
Quantum Physics: YES	Theoretical Physics: YES